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Phononic Crystal Sensor for Detection of D_2O Concentration in H_2O-D_2O Mixture

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Abstract

In this paper, a 2D solid-solid phononic crystal sensor, is proposed to detect D_2O (heavy water) concentration percentage in the range of 90-100% in the H_2O-D_2O mixture. The structure is made of tungsten rods in the aluminum background. To give a resonance mode in the band diagram curve, a cavity region in throughout of a linear waveguide is designed. Finite element method (FEM) is used to calculate and analyse the transmission spectra. H_2O-D_2O mixture with different concentration percentage values of D_2O has added in the cavity region and the acoustic waves behavior is analysed. By changing the D_2O concentration in the mixture, the resonance mode is shifted. Each 1% of D_2O concentration change causes almost 120kHz shift of resonance modes. The performance evaluation process shows the high Q factor and high sensitivity of sensor. The other parameters FOM, SNR, and resolution also show the best performance of proposed structure. This kind of sensors also can be useful to detect the other materials with high efficiency.

Keywords: Phononic crystals; Resonance Mode; Cavity; D_2O (heavy water).

1. Introduction

D_2O or deuterium oxide (often called heavy water) is different from typical light water in its hydrogen's isotope. D_2O has two deuterium atoms instead of two ordinary hydrogens in its molecular formula. Because of this difference in the deuterium and ordinary hydrogens atomic mass, the D_2O is different in the physical properties such as density [1]. Deuterium oxide has numerous applications in industrial and scientific fields such as nuclear magnetic resonance, biological processes, nuclear reactors and as coolant in nuclear power plants [2]. However, because of difference of physical properties between H_2O and D_2O (such as density and speed of sound) we can use phononic crystals (PnCs) in order to efficiently distinguish types of materials or the different compositions of compound materials [3, 4].

PnC is an artificial structure developed to control and manipulate the acoustic waves [5]. They consist of at last two or some material with difference in elasticity, mass density, and longitudinal and transverse velocities of acoustic waves [6].

In the phononic structures, materials can be arranged in one-dimensional (1D), two-dimensional (2D) or three-dimensional (3D) periodicities [7]. In 2015, Aly et al. have introduced a sensor to ionizing particle detection based on 1D structure phononic crystals. Also, in 2019, Mehaney et al. have proposed another 1D structure to neutron detection [8]. However, 2D structures are the popular structures have been investigated in most of structures.

These kinds of sensors are used to detect materials in some works. For example, Gharibi et al. have introduced 2D phononic crystal sensors for sensing propanol [9] and H_2O concentration [3] and heavy metal in water [10]. Also, inside of materials detection, these sensors can be useful in temperature sensing [11]. The 3D structures because of its complex structure have been investigated in a few work [7].

In this paper, we proposed a new method to detect the D_2O percent in H_2O-D_2O mixture based on 2D PnC sensors with high sensitivity. The speed of sound and density of D_2O and H2O in 1 atmosphere at 20°C obtained by Wilsons studies [12]. Finite element method (FEM) is used to calculate transmission spectrum of the incident acoustic wave.

2. Design Procedure

In this work, the 2D phononic crystal is constructed by squire matrix of tungsten rods and aluminium background. scatterer radius (r) is 4mm and lattice constant (a) is 10mm. Table 1 Shows the physical parameter of constituent materials.

In order to calculate the Eigen frequency in the irreducible Brillouin zone (IBZ), the finite element method (FEM) has been used to analyse the unit cell based on Bloch-Floquet theory. For calculating the band diagram, the periodic boundary condition (PBC) should be placed on all boundaries of the structure and wave numbers (Kx, Ky) should be analysed in both ΓX and ΓM directions. Figure 1 shows the unit cell of the structure by the rods of tungsten in the aluminium background.

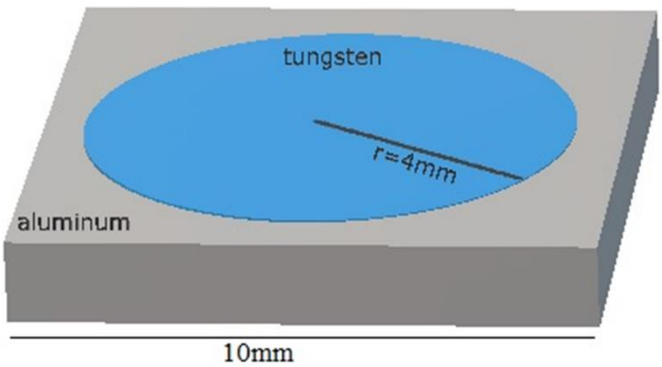

Figure 1. 3D schematics of unit cell.

In order to design of defect mode in the structure, supercell analysis is necessary. As can be seen in Fig. 2(a), we designed 1×5 supercell with a defect in the midst of the structure. The defect consists of two nested hollow cylinders, that inner rod of steel and outer rod of water with 4mm and 4.5mm diameter respectively. Physical parameters of these materials are available in Table 2. Figure 2(b) shows the defect mode by dashed line in the band gap region.

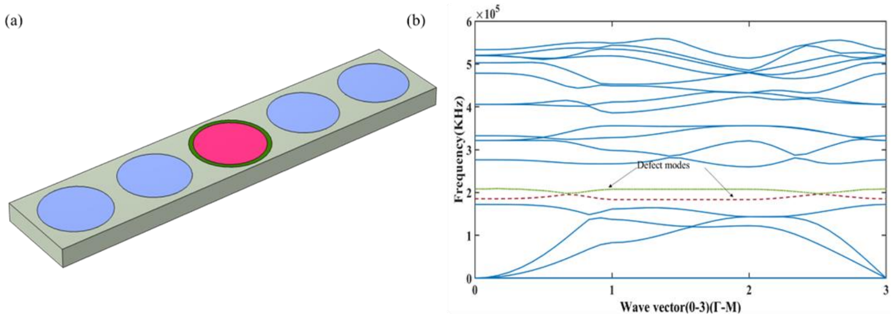

Figure 2. (a) The 3D schematic of super cell. (b) Band structure with two resonance mode (dashed line) in the band gap region.

Table 1. Physical parameter of constituent materials.

material	Mass Density(kg/m^3)	Poison ratio	Young module
aluminium	2700	0.35	70
tungsten	19350	0.28	000

As a mentioned before, D_2O-H_2O mixture is our target sample. At T=20°C, mass density and speed of sound of D_2O are equal to1054kg/m3 and 1483.3 m/s, respectively. The speed of sound and densities of the D_2O-H_2O mixture with different concentrations of D_2O is estimated. A cavity defect is proposed to import acoustic wave to the target sample. To this purpose we need a linier waveguide to import and export acoustic wave to and from cavity region. 2D schematic of complete proposed structure are available in Fig. 3. The size of the rods in the cavity are the same as the waveguide. To achieve the maximum resonance of the sound wave inside the cavity and its interaction with the target sample, the rods on the right and left sides of the cavity were shifted inwards by 0.5 mm.

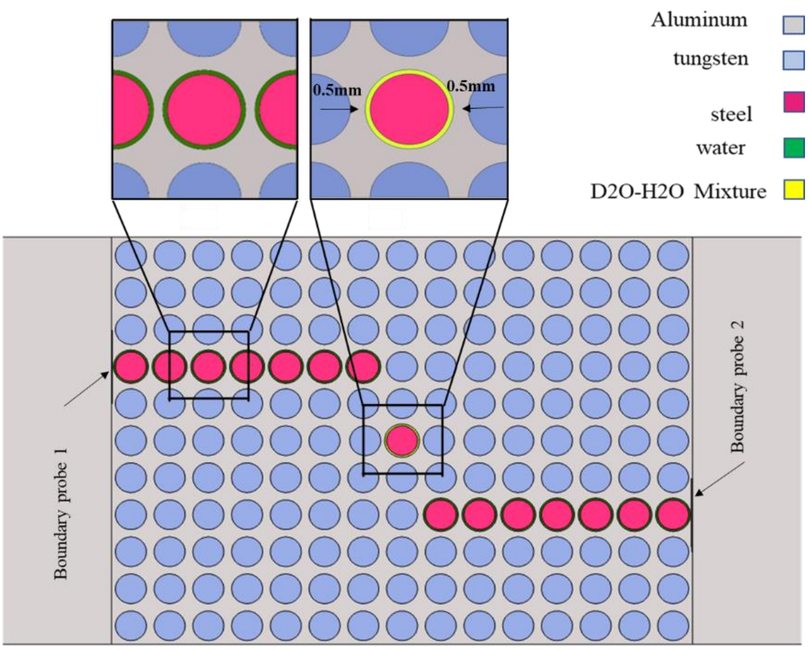

Figure 3. 2D shape of complete structure.

Table 2. Physical parameter of constituent materials.

material	Mass Density(kg/m^3)	Speed of sound	Poison ratio	Young module
Stainless steel	7780	-	0.28	210
water	993	1483	-	-

The structure behaviour while insert sample in cavity and its transmission spectrum is discussed in the next section.

3. Results

Figure 4 shows the resonance peaks related to the percentage of different concentrations of D_2O in the mixture in the range of 90-100% concentration. we have two resonance mode for each concentration percentage. But the high amplitude resonance can be more practical and we chose it to our purpose. Because of long distance between peaks and their extreme sharpness, it is clear this sensor has ability to sense the sample with high precision and minimum changes in the concentration can be traced by sensor.

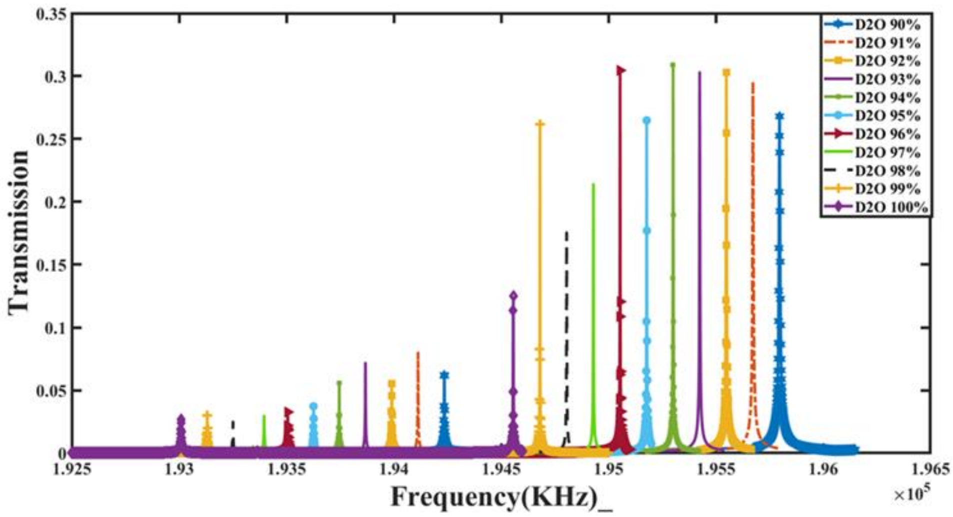

Figure 4. Transmission spectrum for different concentrations of D_2O in water (90% to 100%).

There are some parameters to analyse the performance of sensors [3]. One of these parameters is sensitivity, that calculated by the following relation [3]:

$$. \quad s = \frac{\nabla f}{\nabla x} \tag{1}$$

where ∇f is the resonant frequency difference between each D_2O concentration and zero concentration percentage as $\nabla f = f_{n\%} - f_{0\%}$ and $\nabla \chi$ is the concentration difference. The resonance of zero concentration (water) is taken as a base frequency. Another important parameter is, the quality factor (Qf), which can be calculated by the following relation, where $\nabla f_{1/2}$ is the full width at half maximum (FWHM) of resonance mode [3]:

$$Qf = \frac{f_r}{f_{1/2}} \tag{2}$$

The relation depicted below are figure of merit (FOM) and signal-to-noise ratio (SNR). They are important parameters for any sensor platform as well [3]:

$$FOM = \frac{S}{\nabla f_{1/2}} \tag{3}$$

$$SNR = \frac{\nabla f}{\nabla f_{1/2}} \tag{4}$$

Finally, the sensor resolution (R) is given by the following equation [3]:

$$R = \frac{f_r}{Qf} \tag{5}$$

The performance parameters of proposed sensor are listed in Table 3. The parameter demonstrates very high performance of the proposed sensor.

Table 3. The performance parameters of the D_2O PnC sensor (90% to 100%).

Concentration%	Resonance frequency KHz	Sensitivity Hz	FWHM Hz	Quality-factor	FOM	SNR	R_{Hz}
90	195.797	12415.5	7.4	26459	1677.7	1510	7.4
91	195673	12415.5	5.2	37629	2387.5	2172.6	5.2
92	195549	12415.2	3.9	50140.7	3183.3	2928.7	3.9
93	195425	12415.05	3	65141.6	4138.35	3848.6	3
94	195301	12414.8	2.35	83106.8	5282.8	4965.9	2.35
95	195178	12413.6	2.33	83767.3	5327.7	5061.3	2.33
96	195054	12413.5	1.6	121908.75	7758.43	7448.1	1.6
97	194930	12413.4	1.2	162441.6	10344.5	10034.1	1.2
98	194805	12414.2	2.33	83607.2	5327.9	5221.4	2.33
99	194681	12414.1	1.4	139057.8	8867.2	8778.5	1.4
100(D2O)	194556	12415	2.6	74829.2	4775	4775	2.6

As can be seen in Table 3, the Qf in 99% concentration percentage of D_2O is 139057.8 and sensitivity in all concentration percentages are more than 12413.5. it is clear from these parameters our proposed sensor is capable to detect very small amount of D_2O in the mixture.

4. Conclusions

2D cavity mode phononic crystal sensor proposed for measuring D_2O concentration percentage in the H_2O-D_2O mixture. Finite element method was used for acoustic wave analysis. The resonance peak in the band gap region has frequency shift by D_2O concentration change. The distance between two resonance peaks for each 1% concentration change, almost is 120KHz. The results show high sensitivities and performance of this structure that demonstrate our sensors capability in sensing process. because of low cost and simple process of manufacturing and sensing; this method can be replaced with other complicated methods.

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